Bench
859503

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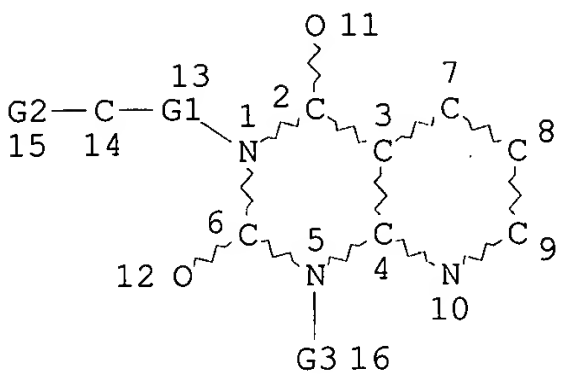


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VAR G3=H/ME/ET
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  16

STEREO ATTRIBUTES: NONE
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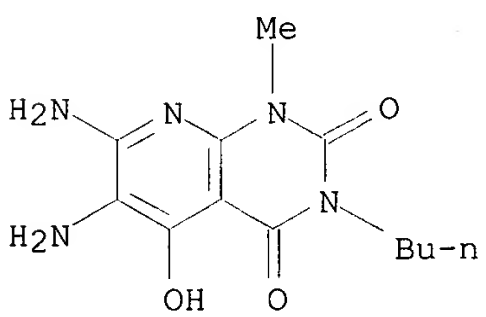
L3 ANSWER 1 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 352225-36-6 REGISTRY
CN Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, 6,7-diamino-3-butyl-5-hydroxy-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H17 N5 O3
SR Chemical Library

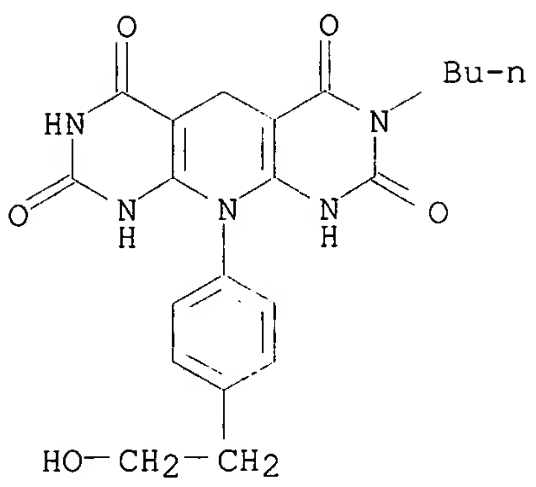


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 ANSWER 2 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 344436-69-7 REGISTRY
CN Pyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetrone, 3-butyl-5,10-dihydro-10-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16

FS 3D CONCORD
MF C21 H23 N5 O5
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

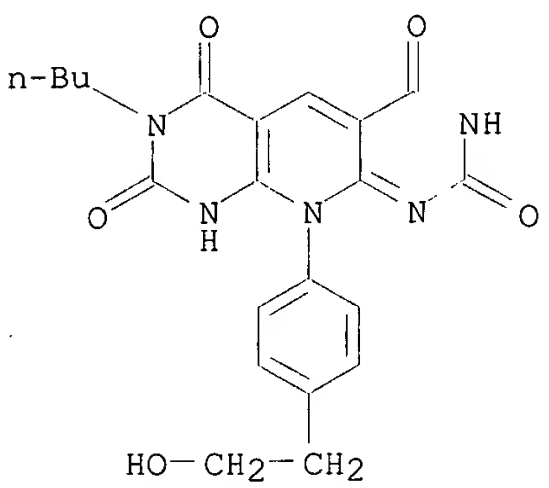
REFERENCE 1: 135:41772 Fluorophore-oligonucleotide-4-(phenyldiazenyl)phenylamine quencher conjugates for use in hybridization assays. Reed, Michael W.; Lukhtanov, Eugeny Alexander; Gall, Alexander A.; Dempcy, Robert O. (Epoch Biosciences, Inc., USA). PCT Int. Appl. WO 2001042505 A2 20010614, 122 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US33333 20001208. PRIORITY: US 1999-457616 19991208.

AB Oligonucleotide-fluorophore-quencher conjugates wherein the fluorophore moiety has emission wavelengths in the range of about (300) to about (800) nm, and or where the quencher includes a substituted 4-(phenyldiazenyl)phenylamine structure provide improved signal to noise ratios and other advantageous characteristics in hybridization and related assays. The oligonucleotide-fluorophore-quencher conjugates can be synthesized by utilizing novel phosphoramidite reagents that incorporate the quencher moiety based on the substituted 4-(phenyldiazenyl)phenylamine structure, and or novel phosphoramidite reagents that incorporate a fluorophore moiety based on the substituted coumarin, substituted 7-hydroxy-3H-phenoxazin-3-one, or substituted 5,10-dihydro-10-[phenyl]pyrido[2,3-d;6,5-d']dipyrimidine-2,4,6,8-(1H,3H,7H,9H,10H)-tetrone structure. Oligonucleotide-fluorophore-quencher-minor groove binder conjugates including a pyrrolo[4,5-e]indolin-7-yl-carbonyl{pyrrolo[4,5-e]indolin-7-yl}carbonyl pyrrolo[,5-e]indoline-7-carboxylate (DPI3) moiety as the minor groove binder and the substituted 4-(phenyldiazenyl)phenylamine moiety as the quencher, were synthesized and have substantially improved hybridization and signal to noise ratio properties.

L3 ANSWER 3 OF 23 REGISTRY COPYRIGHT 2001 ACS

Searched by: Mary Hale 308-4258 CM-1 12D16

RN 344436-68-6 REGISTRY
CN Pyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,10H)-tetrone, 3-butyl-10-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H21 N5 O5
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:41772 Fluorophore-oligonucleotide-4-(phenyldiazenyl)phenylamine quencher conjugates for use in hybridization assays. Reed, Michael W.; Lukhtanov, Eugeny Alexander; Gall, Alexander A.; Dempcy, Robert O. (Epoch Biosciences, Inc., USA). PCT Int. Appl. WO 2001042505 A2 20010614, 122 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US33333 20001208. PRIORITY: US 1999-457616 19991208.

AB Oligonucleotide-fluorophore-quencher conjugates wherein the fluorophore moiety has emission wavelengths in the range of about (300) to about (800) nm, and or where the quencher includes a substituted 4-(phenyldiazenyl)phenylamine structure provide improved signal to noise ratios and other advantageous characteristics in hybridization and related assays. The oligonucleotide-fluorophore-quencher conjugates can be synthesized by utilizing novel phosphoramidite reagents that incorporate the quencher moiety based on the substituted 4-(phenyldiazenyl)phenylamine structure, and or novel phosphoramidite reagents that incorporate a fluorophore moiety based on the substituted coumarin, substituted 7-hydroxy-3H-phenoxazin-3-one, or substituted 5,10-dihydro-10-[phenyl]pyrido[2,3-d;6,5-d']dipyrimidine-2,4,6,8-(1H,3H,7H,9H,10H)-tetrone structure. Oligonucleotide-fluorophore-quencher-minor groove binder conjugates including a pyrrolo[4,5-e]indolin-7-yl-carbonyl{pyrrolo[4,5-e]indolin-7-yl}carbonyl pyrrolo[,5-e]indoline-7-carboxylate (DPI3) moiety as the minor groove binder and the substituted 4-(phenyldiazenyl)phenylamine moiety as the quencher, were synthesized and have substantially improved hybridization and signal to noise ratio

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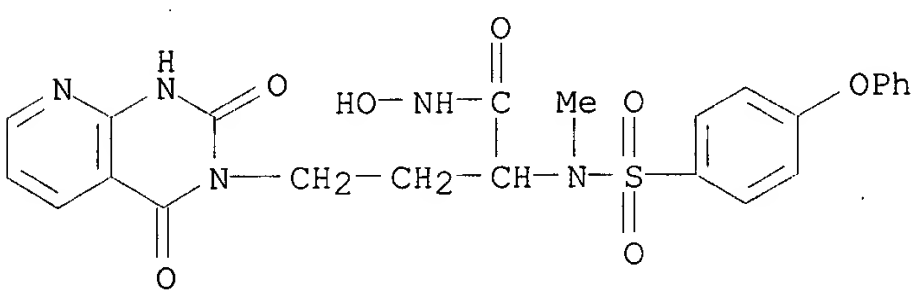
properties.

L3 ANSWER 4 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 246263-35-4 REGISTRY
CN Pyrido[2,3-d]pyrimidine-3(2H)-butanamide, 1,4-dihydro-N-hydroxy-.alpha.-[methyl[(4-phenoxyphenyl)sulfonyl]amino]-2,4-dioxo- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H23 N5 O7 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, TOXLIT

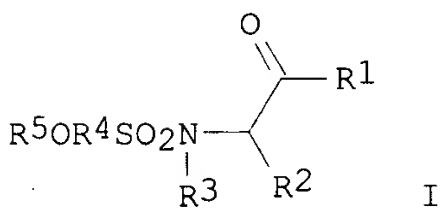


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:56063 Sulfonamide derivatives as matrix metalloproteinase inhibitors. Kimura, Tomio; Miyazaki, Shojiro; Ueda, Keishi; Tanzawa, Kazuhiko; Ushiyama, Shigeru; Takasaki, Wataru (Sankyo Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2001163786 A2 20010619, 120 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2000-297744 20000929. PRIORITY: JP 1999-278300 19990930.

GI



I

AB The sulfonamide derivs. (I; R1 = H, NHOH; R2 = H, (substituted)alkyl, cycloalkyl, -AR6 [A = O, -S(O)m- or -n(R9)- with alkylene; R6 = other groups]; R3 = H, (substituted)-alkyl, -cycloalkyl, -alkenyl, and -alkynyl; R4 = (substituted)(hetero)arylene; R5 = (substituted)-alkyl and -(hetero)aryl) and their pharmacol. acceptable salts are claimed as matrix metalloproteinase inhibitors for treatment of arthritis, rheumatoid arthritis, cancer metastasis, and breast cancer.

REFERENCE 2: 131:286264 Preparation of phenylsulfonamide derivatives as proteinase and aggrecanase inhibitors. Kimura, Tomio; Miyazaki, Shoujiro; Ueda, Keiji; Tanzawa, Kazuhiko; Ushiyama, Shigeru; Takasaki, Wataru (Sankyo Company, Limited, Japan). PCT Int. Appl. WO 9951572 A1 19991014, 285 pp. DESIGNATED STATES: W: AU, BR, CA, CN, CZ, HU, ID, IL, IN, KR, MX, NO, NZ, PL, PT, RU, TR, US, ZA; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (Japanese). CODEN: PIXXD2. APPLICATION: WO 1999-JP1751 19990402. PRIORITY: JP 1998-91819 19980403;

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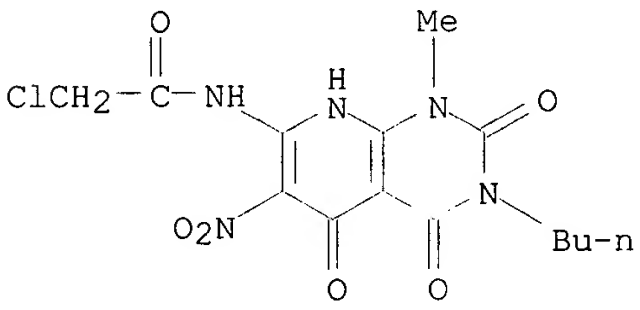
JP 1999-53164 19990301.

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. R5OR4SO2N(R3)CH(R2)COR1 [I; wherein R1 is H or NHOH; R2 is H, optionally substituted alkyl, cycloalkyl, or AR6 (wherein A is O, S(O)m, or alkylene optionally interrupted by N(R9); and R6 is a group represented by Q, Q1, Q2 wherein X is O, S, N(R10), or C(R11)(R12); Y is O, CO, S(O)n, N(R10), or C(R11)(R12); R7 and R8 each is H, alkyl, COOH, optionally substituted alkyl, etc.; R9, R10, R11, and R12 each is H, alkyl, etc.; and m and n each is 0 to 2); R3 is H, optionally substituted alkyl, optionally substituted cycloalkyl, optionally substituted alkenyl, or optionally substituted alkynyl; R4 is optionally substituted (hetero)arylene; and R5 is optionally substituted alkyl or optionally substituted (hetero)aryl], stereoisomers, pharmacol. acceptable salts, esters, or other derivs. thereof are prepd. and tested as matrix metalloproteinase-13 inhibitors and aggrecanase inhibitors. Thus, the title compd. II was prepd.

L3 ANSWER 5 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 177952-56-6 REGISTRY
CN Acetamide, N-(3-butyl-1,2,3,4,5,8-hexahydro-1-methyl-6-nitro-2,4,5-trioxopyrido[2,3-d]pyrimidin-7-yl)-2-chloro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H16 Cl N5 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

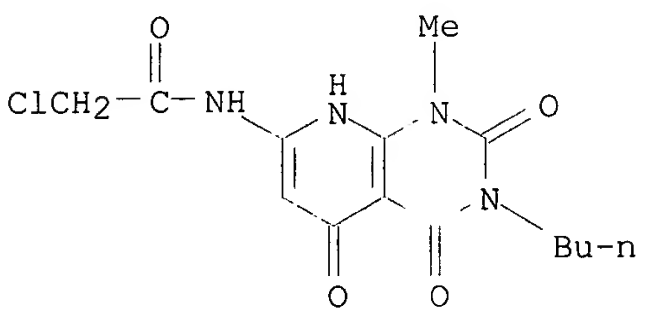
REFERENCE 1: 125:48741 Synthesis and diuretic activity of 7-acylaminopyrido[2,3-d]pyrimidine-2,4,5-triones. Burova, O. A.; Skudamova, T. I.; Burov, D. M.; Smirnova, N. M.; Romanova, T. V.; Safonova, T. S. (NIKhFI, Novokuznetsk, Russia). Khim.-Farm. Zh., 28(11), 25-28 (Russian) 1994. CODEN: KHFZAN. ISSN: 0023-1134.

AB A no. of 7-acylamino-, 6-bromo-, and 6-nitro-7-acylaminopyrido[2,3-d]pyrimidine-2,4,5-triones were synthesized and tested for their biol. activity. Some of the compds. had diuretic effects in rats.

L3 ANSWER 6 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 177952-47-5 REGISTRY
CN Acetamide, N-(3-butyl-1,2,3,4,5,8-hexahydro-1-methyl-2,4,5-trioxopyrido[2,3-d]pyrimidin-7-yl)-2-chloro- (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16

FS 3D CONCORD
MF C14 H17 Cl N4 O4
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



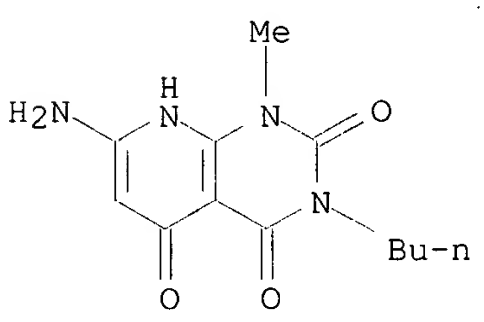
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:48741 Synthesis and diuretic activity of 7-acylaminopyrido[2,3-d]pyrimidine-2,4,5-triones. Burova, O. A.; Skudamova, T. I.; Burov, D. M.; Smirnova, N. M.; Romanova, T. V.; Safonova, T. S. (NIKhFI, Novokuznetsk, Russia). Khim.-Farm. Zh., 28(11), 25-28 (Russian) 1994. CODEN: KHFZAN. ISSN: 0023-1134.

AB A no. of 7-acylamino-, 6-bromo-, and 6-nitro-7-acylaminopyrido[2,3-d]pyrimidine-2,4,5-triones were synthesized and tested for their biol. activity. Some of the compds. had diuretic effects in rats.

L3 ANSWER 7 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 177952-42-0 REGISTRY
CN Pyrido[2,3-d]pyrimidine-2,4,5(1H,3H,8H)-trione, 7-amino-3-butyl-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H16 N4 O3
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:48741 Synthesis and diuretic activity of 7-acylaminopyrido[2,3-d]pyrimidine-2,4,5-triones. Burova, O. A.; Skudamova, T. I.; Burov, D. M.; Smirnova, N. M.; Romanova, T. V.; Safonova, T. S. (NIKhFI, Novokuznetsk, Russia). Khim.-Farm. Zh., 28(11), 25-28 (Russian) 1994. CODEN: KHFZAN. ISSN: 0023-1134.

Searched by: Mary Hale 308-4258 CM-1 12D16

AB A no. of 7-acylamino-, 6-bromo-, and 6-nitro-7-acylaminopyrido[2,3-d]pyrimidine-2,4,5-triones were synthesized and tested for their biol. activity. Some of the compds. had diuretic effects in rats.

L3 ANSWER 8 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 140934-38-9 REGISTRY
CN Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, 3-(1,1-dimethyl-2-oxopropyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H13 N3 O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMINFORMRX
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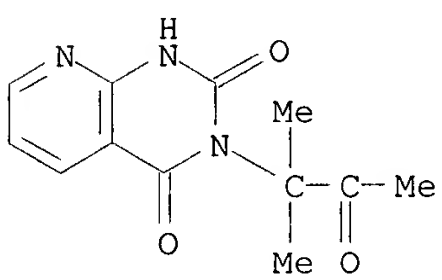
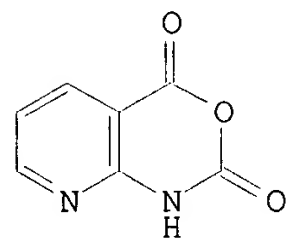


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 116:235563 Acetylenic chemistry. Part 20. Ring opening of 3-azaisatoic anhydride with acetylenic amines: synthesis of pyrido[2,3-d]pyrimidones. Reisch, Johannes; Usifoh, Cyril O.; Oluwadiya, James O. (Inst. Pharm. Chem., Univ. Muenster, Muenster, W-4400, Germany). Monatsh. Chem., 123(3), 247-50 (English) 1992. CODEN: MOCMB7. ISSN: 0026-9247.

GI



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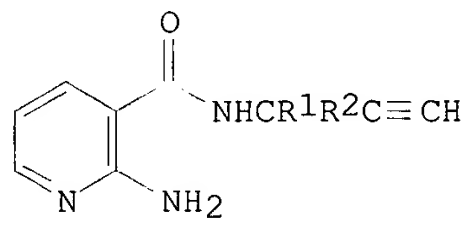

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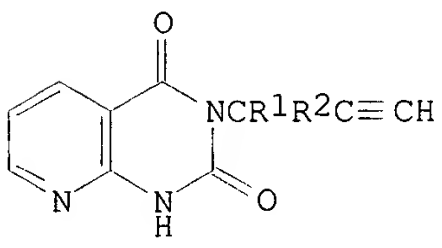

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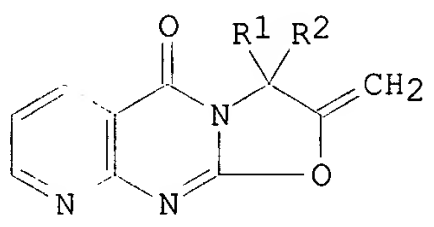
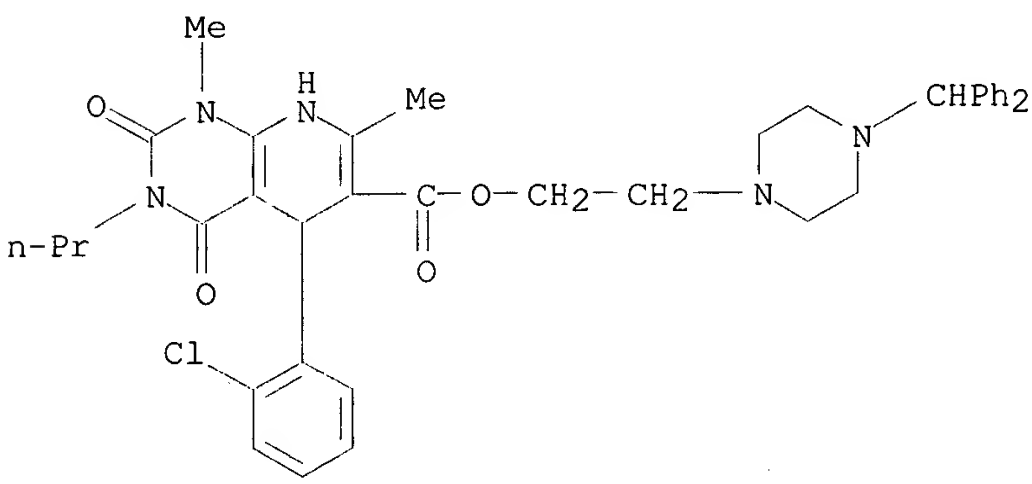


IV

AB Ring opening of 3-azaisatoic anhydride I with acetylenic amines HC.tplbond.CCR1R2NH2 [R1 = R2 = H, Me; R1R2 = (CH2)5] gave the nicotinamides II. The reaction of triphosgene with the nicotinamides II yielded the pyrido[2,3-d]pyrimidinones III (R1 =R2 = H, Me) and oxazolopyridopyrimidinones IV [R1 = R2 = Me; R1R2 = (CH2)5].

Searched by: Mary Hale 308-4258 CM-1 12D16

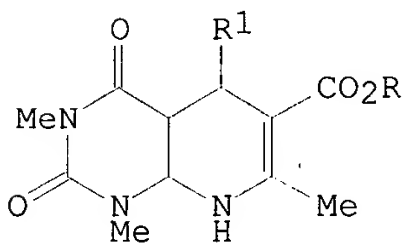
L3 ANSWER 9 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 133689-50-6 REGISTRY
CN Pyrido[2,3-d]pyrimidine-6-carboxylic acid, 5-(2-chlorophenyl)-1,2,3,4,5,8-hexahydro-1,7-dimethyl-2,4-dioxo-3-propyl-, 2-[4-(diphenylmethyl)-1-piperazinyl]ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)
MF C38 H42 Cl N5 O4 . 2 Cl H
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



●2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 114:207192 The Hantzsch synthesis with 6-aminouracils: one step synthesis of pyrido[2,3-d]pyrimidines. Kajino, Masahiro; Meguro, Kanji (Res. Dev. Div., Takeda Chem. Ind., Ltd., Osaka, 532, Japan). Heterocycles, 31(12), 2153-61 (English) 1990. CODEN: HTCYAM. ISSN: 0385-5414.
GI



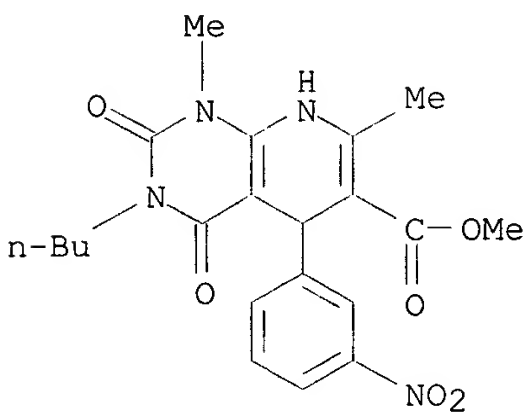
I

AB A one-step synthesis of a new pyrido[2,3-d]pyrimidine derivs., e.g. I [R = Me, Et, (CH2)2NMeCH2Ph, (CH2)2NMePh, R1 = C6H4NO2-3, C6H3Cl2-2,3], was achieved through the Hantzsch synthesis using 6-aminouracils as enamine nucleophiles. Antihypertensive activity of I was evaluated.

L3 ANSWER 10 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 133657-14-4 REGISTRY
CN Pyrido[2,3-d]pyrimidine-6-carboxylic acid, 3-butyl-1,2,3,4,5,8-hexahydro-1,7-dimethyl-5-(3-nitrophenyl)-2,4-dioxo-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD

Searched by: Mary Hale 308-4258 CM-1 12D16

MF C21 H24 N4 O6
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

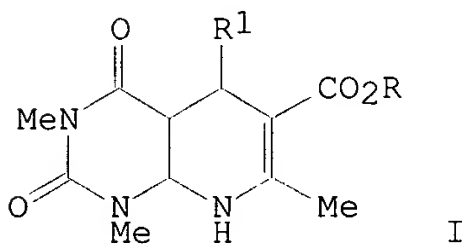


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 114:207192 The Hantzsch synthesis with 6-aminouracils: one step synthesis of pyrido[2,3-d]pyrimidines. Kajino, Masahiro; Meguro, Kanji (Res. Dev. Div., Takeda Chem. Ind., Ltd., Osaka, 532, Japan). Heterocycles, 31(12), 2153-61 (English) 1990. CODEN: HTCYAM. ISSN: 0385-5414.

GI



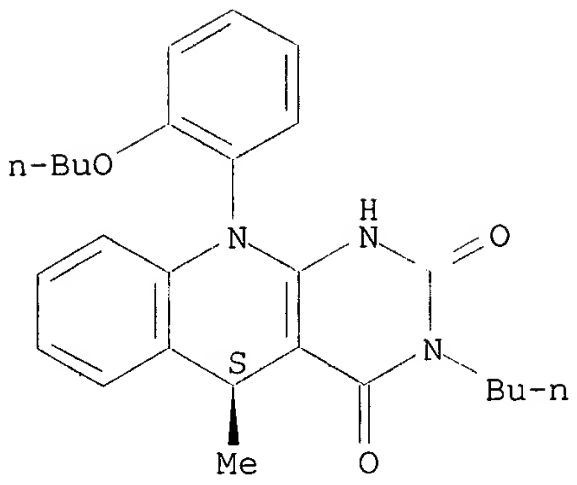
I

AB A one-step synthesis of a new pyrido[2,3-d]pyrimidine derivs., e.g. I [R = Me, Et, (CH2)2NMeCH2Ph, (CH2)2NMePh, R1 = C6H4NO2-3, C6H3Cl2-2,3], was achieved through the Hantzsch synthesis using 6-aminouracils as enamine nucleophiles. Antihypertensive activity of I was evaluated.

L3 ANSWER 11 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 125085-67-8 REGISTRY
CN Pyrimido[4,5-b]quinoline-2,4(1H,3H)-dione, 10-(2-butoxyphenyl)-3-butyl-5,10-dihydro-5-methyl-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H31 N3 O3
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

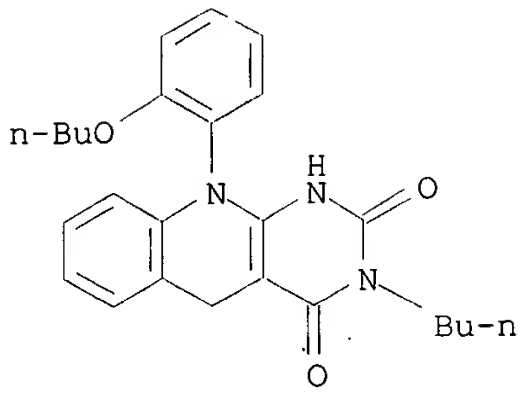
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:72746 Coenzyme models. 51. Structure and reactivity studies of 5-methyl-5-deazaflavinophanes: on the "axial preference" in a flavin redox system. Shinkai, Seiji; Nishiyama, Noriaki; Matsuda, Tsutomu; Kanazawa, Ryusuke; Kawase, Akito; Manabe, Osamu (Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan). Bioorg. Chem., 17(3), 344-58 (English) 1989. CODEN: BOCMBM. ISSN: 0045-2068.

AB Structures and reactivities of 5-deazaflavins were studied by using new 5-deazaflavinophanes dFl(n) in which N(3) and O(2') in the 10-(2-hydroxy)phenyl group were linked by a (CH2)n chain (n = 8 and 12). DFl(Bu), having n-Bu groups at N(3) and O(2'), was used as a ref. X-ray crystallog. and 1H NMR studies established that in the Grignard reaction with MeMgBr to yield dFlMered(n) the Me group attacks the isoalloxazine plane from the axial side and is fixed at the axial position. In NaBH4 redn. of dFlMe(n) to yield dFlMered(n) hydride attacks the isoalloxazine plane from the axial side, but the 5-Me group is displaced from equatorial to axial by ring inversion in order to minimize steric hindrance. The axial preference obsd. for nucleophilic attacks is explained by a stereoelectronic effect. DFlMered(n), having only Heq at the C(5)-position, was much less reactive as reductant than dFlred(n) having both Heq and Hax. The deactivation is rationalized by such that (i) more reactive Hax is lost by substitution with the Me group and (ii) remaining Heq, surrounded by bulky groups, behaves as a less reactive buried hydride equiv. These novel structure-reactivity relationships have important implications on biochem. studies of flavoenzymes.

L3 ANSWER 12 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 125085-66-7 REGISTRY
CN Pyrimido[4,5-b]quinoline-2,4(1H,3H)-dione, 10-(2-butoxyphenyl)-3-butyl-5,10-dihydro- (9CI) (CA INDEX NAME)
MF C25 H29 N3 O3
SR CA
LC STN Files: CA, CAPLUS

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

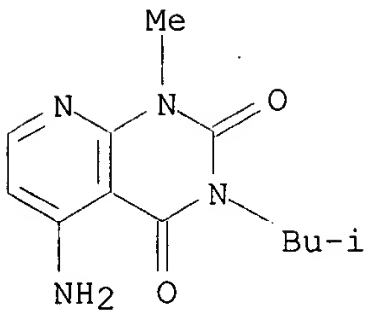
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:72746 Coenzyme models. 51. Structure and reactivity studies of 5-methyl-5-deazaflavinophanes: on the "axial preference" in a flavin redox system. Shinkai, Seiji; Nishiyama, Noriaki; Matsuda, Tsutomu; Kanazawa, Ryusuke; Kawase, Akito; Manabe, Osamu (Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan). Bioorg. Chem., 17(3), 344-58 (English) 1989. CODEN: BOCMBM. ISSN: 0045-2068.

AB Structures and reactivities of 5-deazaflavins were studied by using new 5-deazaflavinophanes dFl(n) in which N(3) and O(2') in the 10-(2-hydroxy)phenyl group were linked by a (CH2)n chain (n = 8 and 12). DFl(Bu), having n-Bu groups at N(3) and O(2'), was used as a ref. X-ray crystallog. and 1H NMR studies established that in the Grignard reaction with MeMgBr to yield dFlMered(n) the Me group attacks the isoalloxazine plane from the axial side and is fixed at the axial position. In NaBH4 redn. of dFlMe(n) to yield dFlMered(n) hydride attacks the isoalloxazine plane from the axial side, but the 5-Me group is displaced from equatorial to axial by ring inversion in order to minimize steric hindrance. The axial preference obsd. for nucleophilic attacks is explained by a stereoelectronic effect. DFlMered(n), having only Heq at the C(5)-position, was much less reactive as reductant than dFlred(n) having both Heq and Hax. The deactivation is rationalized by such that (i) more reactive Hax is lost by substitution with the Me group and (ii) remaining Heq, surrounded by bulky groups, behaves as a less reactive buried hydride equiv. These novel structure-reactivity relationships have important implications on biochem. studies of flavoenzymes.

L3 ANSWER 13 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 112762-11-5 REGISTRY
CN Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, 5-amino-1-methyl-3-(2-methylpropyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H16 N4 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Searched by: Mary Hale 308-4258 CM-1 12D16

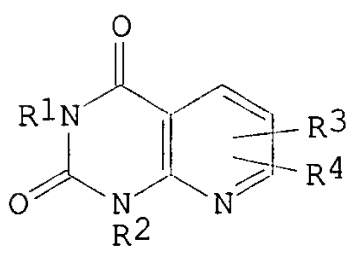


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 108:75422 Preparation of pyrido[2,3-d]pyrimidine derivatives as allergy inhibitors and antiasthmatics. Go, Kouichiro; Kurimoto, Yoshiyuki; Kitamura, Norihiko (Nippon Zoki Pharmaceutical Co., Ltd., Japan). Eur. Pat. Appl. EP 243311 A2 19871028, 36 pp. DESIGNATED STATES: R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1987-810233 19870410. PRIORITY: JP 1986-89064 19860416.

GI

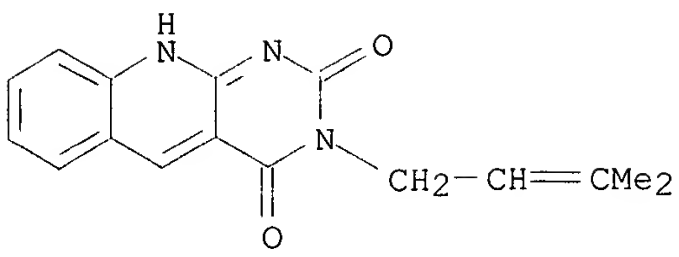


I

AB The title compds. [I; R1, R2 = alkyl; R3, R4 = H, halo, OH, NO2, amino, hydrazino, N3, alkenylamino, (hydroxy-substituted) alkylamino] were prepd. as allergy inhibitors. 5-Acetyl-6-amino-1,3-dimethyluracil and POCl3 were heated in DMF at 60.degree. for 2 h to give 5-chloro-1,3-dimethylpyrido[2,3-d]pyrimidine-2,4-dione, which was hydrogenated in MeOH over Pd/C to give 1,3-dimethylpyrido[2,3-d]pyrimidine-2,4-dione (II). II at 20 mg/kg orally gave 51.2% inhibition of passive cutaneous anaphylaxis in rats.

L3 ANSWER 14 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 112499-57-7 REGISTRY
CN Pyrimido[4,5-b]quinoline-2,4(1H,3H)-dione, 3-(3-methyl-2-butenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H15 N3 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Searched by: Mary Hale 308-4258 CM-1 12D16

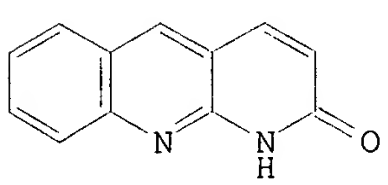


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

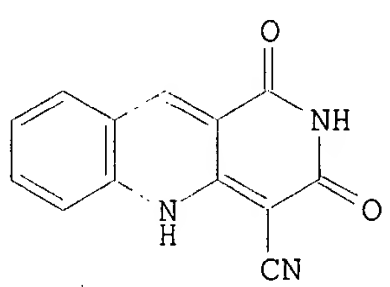
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 108:55932 Friedlaender condensations of o-aminobenzaldehyde with hydroxypyridines. Reisch, Johannes; Scheer, Mathias (Inst. Pharm. Chem., Univ. Muenster, Muenster, D-4400, Fed. Rep. Ger.). Arch. Pharm. (Weinheim, Ger.), 320(11), 1174-80 (German) 1987. CODEN: ARPMAS. ISSN: 0365-6233.

GI



II

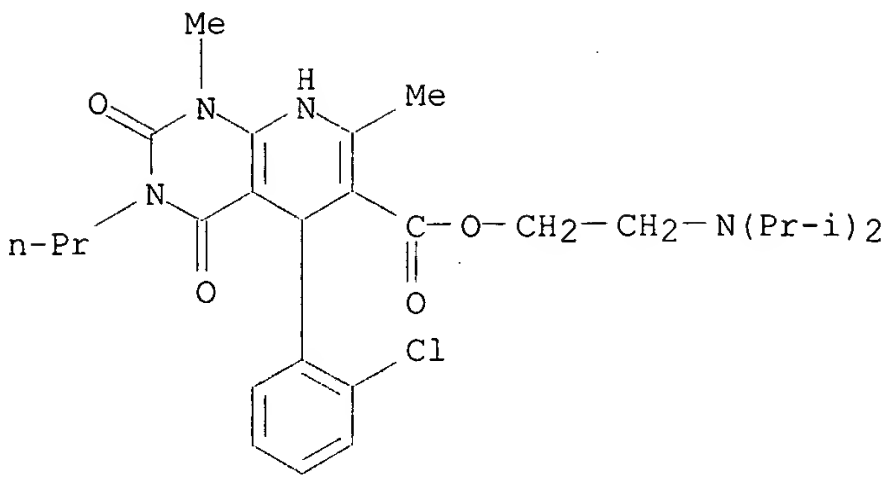


III

AB Condensation reactions of o-H2NC6H4CHO (I) with 2,6-dihydroxypyridine under Friedlaender conditions result in the formation of benzo[b][1,8]naphthyridine II. Reaction of I with 2,4,6-trihydroxypyridine-3-carbonitrile yields the expected dioxobenzo[b][1,6]naphthyridinecarbonitrile III. 4-Hydroxy-2(1H)-oxobenzo[b][1,8]naphthyridine-3-carbonitrile is also isolated. N-methylation and substitution of the ring systems with alkyl groups are also reported.

L3 ANSWER 15 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 96996-29-1 REGISTRY
CN Pyrido[2,3-d]pyrimidine-6-carboxylic acid, 5-(2-chlorophenyl)-1,2,3,4,5,8-hexahydro-1,7-dimethyl-2,4-dioxo-3-propyl-, 2-[bis(1-methylethyl)amino]ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H37 Cl N4 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16

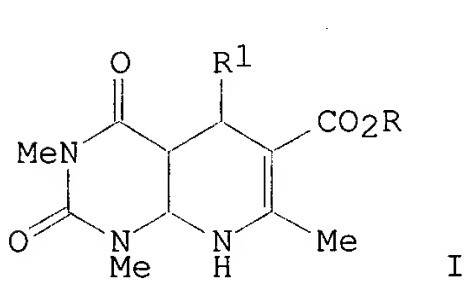


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 114:207192 The Hantzsch synthesis with 6-aminouracils: one step synthesis of pyrido[2,3-d]pyrimidines. Kajino, Masahiro; Meguro, Kanji (Res. Dev. Div., Takeda Chem. Ind., Ltd., Osaka, 532, Japan). Heterocycles, 31(12), 2153-61 (English) 1990. CODEN: HTCYAM. ISSN: 0385-5414.

GI

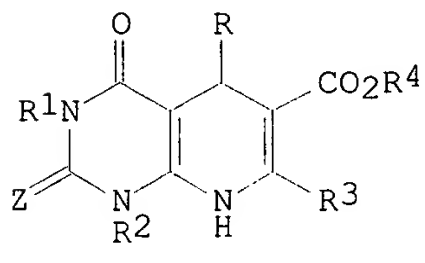


I

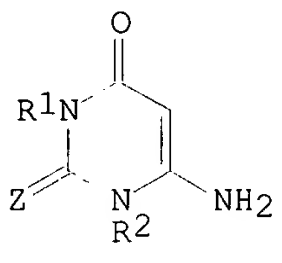
AB A one-step synthesis of a new pyrido[2,3-d]pyrimidine derivs., e.g. I [R = Me, Et, (CH2)2NMeCH2Ph, (CH2)2NMePh, R1 = C6H4NO2-3, C6H3Cl2-2,3], was achieved through the Hantzsch synthesis using 6-aminouracils as enamine nucleophiles. Antihypertensive activity of I was evaluated.

REFERENCE 2: 103:22612 Pyridopyrimidine derivatives. (Takeda Chemical Industries, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 59225188 A2 19841218 Showa, 8 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1983-99210 19830602.

GI



I

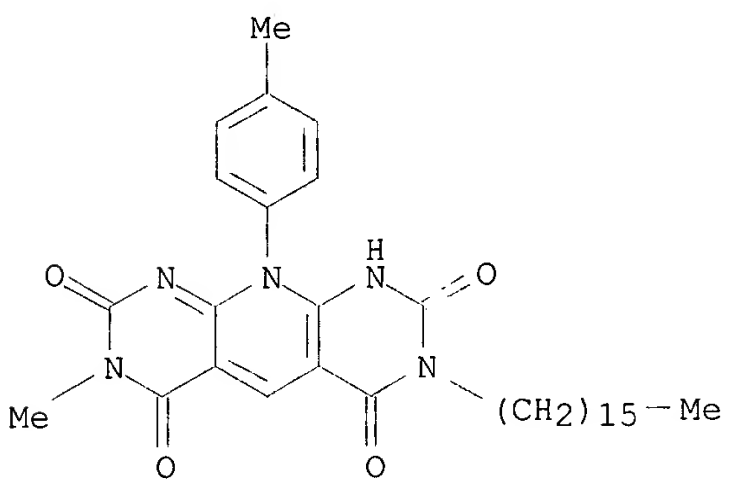


II

Searched by: Mary Hale 308-4258 CM-1 12D16

AB Forty-one pyridopyrimidine derivs. I [R = (un)substituted Ph; R1, R2, R3 = H, alkyl; R4 = (un)substituted alkyl; Z = O, S] were prepd. by reaction of II with RCH:C(CO2R4)(COR3) (III). Hypotensive test data of I were shown in pentobarbital Na-anesthetic dogs and rats. Thus, a mixt. of 2.89 g II (R1 = R2 = Me, Z = O) and 4.65 g III (R = 3-O2NC6H4, R3 = R4 = Me) in EtOH was refluxed 3 h to give 87.4% I (R = 3-O2NC6H4, R1 = R2 = R3 = R4 = Me; Z = O).

L3 ANSWER 16 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 85194-64-5 REGISTRY
CN Pyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,10H)-tetrone, 3-hexadecyl-7-methyl-10-(4-methylphenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C33 H45 N5 O4
LC STN Files: CA, CAPLUS

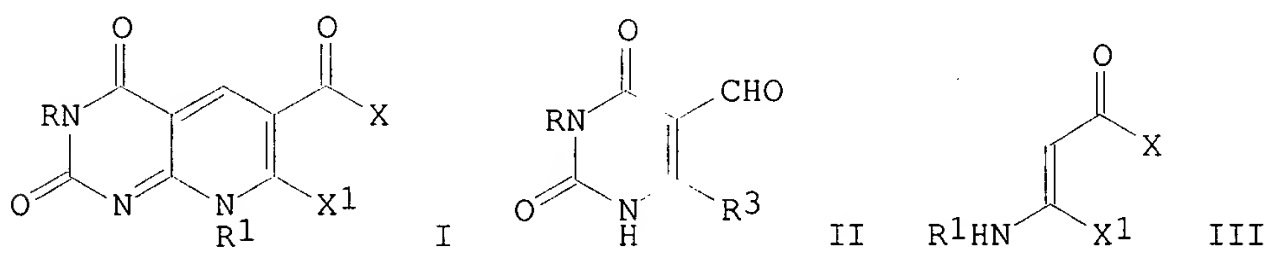


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 98:143450 Pyridodipyrimidine derivatives. (Takeda Chemical Industries, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 57163379 A2 19821007 Showa, 8 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1981-48726 19810331.

GI

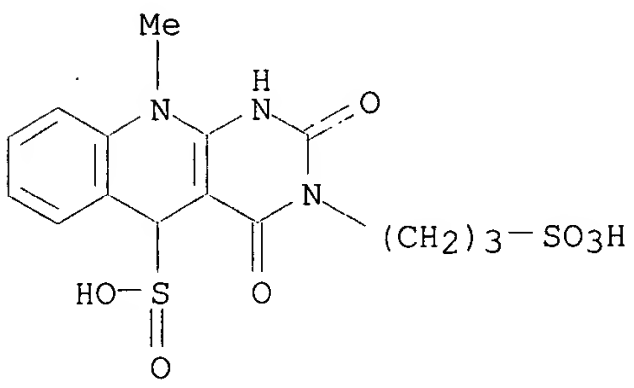


AB Thirty-eight pyridodipyrimidines (I, R, R1, R2 = alkyl, aralkyl, aryl; X-X1 = NR2CONH, NHCR2:N) were prepd. by reaction of II (R3 = halo) with III. I are useful as oxidizing agents. Thus, refluxing 1.13 g II (R = Me, R3 = Cl) with 0.78 g III (R1 = Me, X-X1 = NMeCONH) in AcOH 5 h gave 76% I (R = R1 = Me, X-X1 = NMeCONH).

L3 ANSWER 17 OF 23 REGISTRY COPYRIGHT 2001 ACS

Searched by: Mary Hale 308-4258 CM-1 12D16

RN 73116-42-4 REGISTRY
CN Pyrimido[4,5-b]quinoline-3(2H)-propanesulfonic acid, 1,4,5,10-tetrahydro-10-methyl-2,4-dioxo-5-sulfino- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H17 N3 O7 S2
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

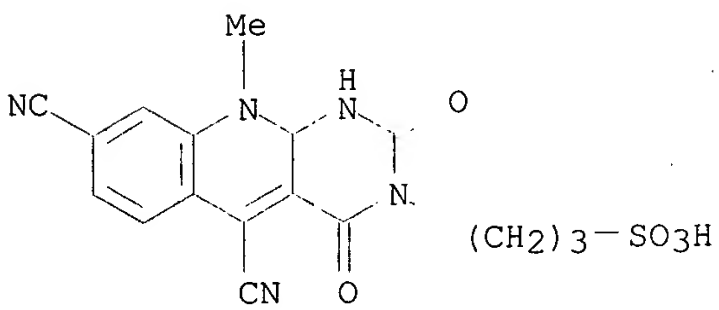
REFERENCE 1: 92:123579 Sulfoxylate ion (HSO2-), the hydride donor in dithionite-dependent reduction of NAD+ analogs. Blankenhorn, Gunter; Moore, Edwin G. (Fachber. Biol., Univ. Konstanz, Konstanz, Fed. Rep. Ger.). J. Am. Chem. Soc., 102(3), 1092-8 (English) 1980. CODEN: JACSAT. ISSN: 0002-7863.

AB At high pH interaction of dithionite with NAD analogs resulted in formation of a sulfinate adduct. Its rate of formation was linearly dependent on dithionite concn. Hence, sulfinate radicals do not appear to be involved in this process. A linear free energy relation for adduct formation was obtained, the rate of which increased with increasing redox potential of the NAD analog. The deprotonated adducts were very stable both thermodynamically (Kd <10-7M) and kinetically (Koff <10-4 s-1). Formation of NADH analogs is therefore not obsd. at pH >11. Conversion of adducts, formed from stoichiometric amts. of NAD analog and dithionite at high pH, to NADH analog was studied by pH jump, stopped-flow spectrophotometry. After protonation of the sulfinate function, formation of oxidized NAD analog was obsd. in a fast initial phase (k for NAD = 4.62 s-1), the rate of which increased with decreasing redox potential of nicotinamide. In a much slower, 2nd phase, formation of NADH analog was obsd., which took >20 min to completion. NADH formation was prevented by adding HCHO which traps the active reducing species. If NAD sulfinate was mixed a pH 5 with an equimolar amt. of the high-potential analog 3-acetylpyridine-NAD, almost quant. formation of 3-acetylpyridine-NADH was obsd. with no detectable formation of NADH. Apparently, sulfoxylate ion (HSO2-), a hydride donor formed after heterolytic dissocn. of the protonated sulfinate adduct, is the active reducing species. Neither the sulfinate adduct itself nor sulfinate radicals appear to be productive in NADH formation. Hence, dithionite appears to be a selective, ambivalent reducing agent. The factors controlling the nicotinamide pathway are both the high thermodn. instability of the nicotinamide radical and the stability of the sulfinate adduct.

L3 ANSWER 18 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 64630-14-4 REGISTRY
CN Pyrimido[4,5-b]quinoline-3(2H)-propanesulfonic acid, 5,8-dicyano-1,4,10,10a-tetrahydro-10-methyl-2,4-dioxo- (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 12D16

FS 3D CONCORD
MF C17 H15 N5 O5 S
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

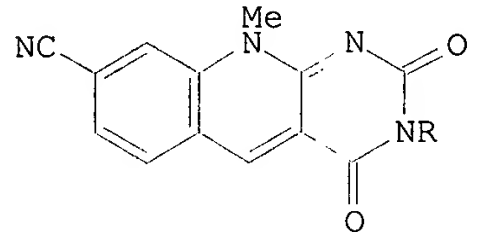


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

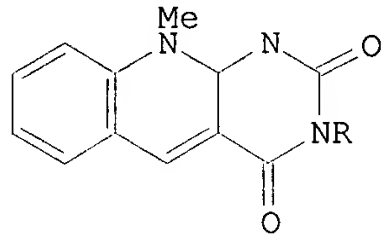
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 87:200420 The chemistry of an electron-deficient 5-deazaflavin. 8-Cyano-10-methyl-5-deazaisoalloxazine. Chan, Rebecca L.; Bruice, Thomas C. (Dep. Chem., Univ. California, Santa Barbara, Calif., USA). J. Am. Chem. Soc., 99(20), 6721-30 (English) 1977. CODEN: JACSAT.

GI



I



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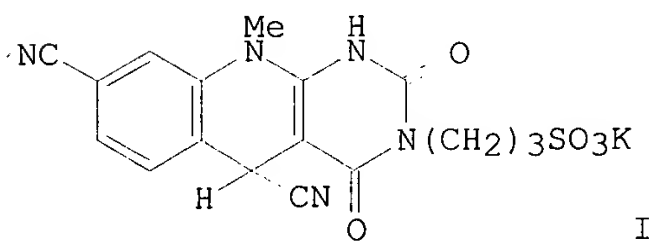

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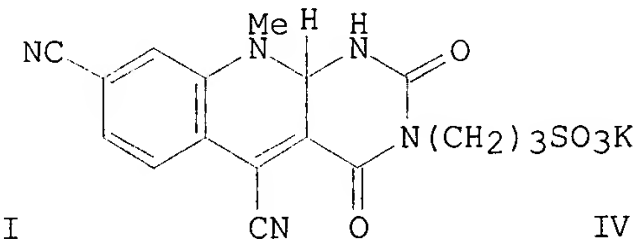
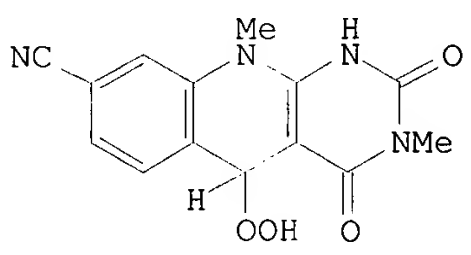


IV



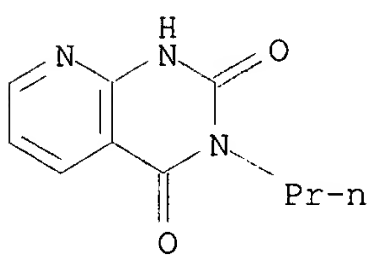
V

AB The syntheses of 8-cyano-3-R-10-methyl-5-deazaisoalloxazines [I; R = Me, PrSO3H] are described, as is a comparison of the reactions of I and 3-R-10-methyl-5-deazaisoalloxazine [I; R = Me, (CH2)3SO3K] with a no. of nucleophiles. Thiolate anions, SO32-, HSO3-, CN-, HO- and HO2- add to the 5 position of I. Though RS- species provide no detectable reaction with II, the pseudo-1st-order rate consts. for addn. to I exceed 170 s-1. The formation equil. consts. for HSCH2CH2OH and dithiothreitol were 490 and 1800 M-1, resp. The 2nd-order rate consts. and addn. equil. consts. for

Searched by: Mary Hale 308-4258 CM-1 12D16

SO32-, HO- and CN- to I exceed those consts. detd. with II by 10-100. Reaction of CN- with I is characterized by a consecutive pseudo-1st-order A .fwdarw. B .fwdarw. C process. The intermediate B represents the C acid III derived by addn. of CN- to the 5 position of I. OH--mediated 1,3-prototropic shift converts III to 5,8-dicyano-1,10a-dihydro-10-methyl-5-deazaisoalloxazine (IV). The C acid IV has pKa 4.5 for dissocn. of the 10a proton, owing to resonance stabilization of the electron pair of the carbanion to both 5- and 8-cyano groups. 8-Cyano-1,5-dihydro-5-hydroperoxy-3,10-dimethyl-5-deazaisoalloxazine (V), obtained on reaction of H2O2 with I, oxidizes I- to I3- with a 2nd-order rate const. 600 times greater than that detd. for the oxidn. of I- by Me3COOH.

L3 ANSWER 19 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 62260-89-3 REGISTRY
CN Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, 3-propyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H11 N3 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

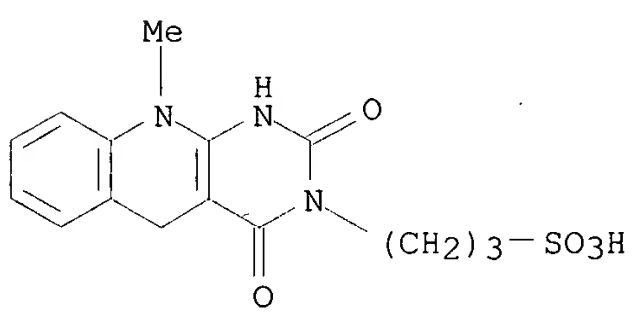


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:121288 Synthesis and properties of 2,4-dioxo-3-R-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidines. Mikhalev, A. I.; Kozhevnikov, Yu. V.; Konshin, M. E. (USSR). Tr. Perm. S.-kh. In-t (118), 57-9 From: Ref. Zh., Khim. 1976, Abstr. No. 23Zh223 (Russian) 1976.
AB Title only translated.

L3 ANSWER 20 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 60397-03-7 REGISTRY
CN Pyrimido[4,5-b]quinoline-3(2H)-propanesulfonic acid, 1,4,5,10-tetrahydro-10-methyl-2,4-dioxo- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H17 N3 O5 S
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



Searched by: Mary Hale 308-4258 CM-1 12D16

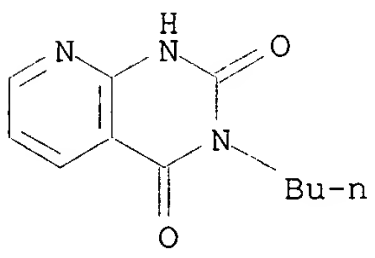
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 85:105973 Nicotinamide-dependent one-electron and two-electron (flavin) oxidoreduction: thermodynamics, kinetics, and mechanism. Blankenhorn, Gunter (Fachber. Biol., Univ. Konstanz, Constance, Ger.). Eur. J. Biochem., 67(1), 67-80 (English) 1976. CODEN: EJBCAI.

AB Biol. nicotinamide-dependent oxidoreduction consists of reversible 2e- oxidoreduction of substrates. A mechanism involving subsequent 1e- steps is shown to be very unfavorable because of the high energy of the nicotinamide radical. Free energy relations provide a convenient tool, allowing differentiation between hydride transfer and H atom transfer. Thus, biol. nicotinamide-dependent, as well as flavine-nicotinamide oxidoreduction, proceed via hydride transfer but not via H atom transfer. In flavine-nicotinamide oxidoreduction, flavine-nicotinamide charge transfer complexes are very likely the catalytic intermediates, preceding transfer of hydride ion. The energy of the long-wavelength charge transfer transition of zwitterionic oxidized nicotinamide-reduced-flavine complexes is strongly dependent on polarity. It is max. in a highly polar environment. 5-Deazaflavines show the high thermodn. radical instability of nicotinamides. They have to be considered as nicotinamide analog 2e- oxidoreductants rather than flavine analogs, therefore, lacking the ability to catalyze reversible 1e- oxidoreduction, essential for many flavoenzymes.

L3 ANSWER 21 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 56788-15-9 REGISTRY
CN Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, 3-butyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H13 N3 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1967 TO DATE)
4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:121288 Synthesis and properties of 2,4-dioxo-3-R-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidines. Mikhalev, A. I.; Kozhevnikov, Yu. V.; Konshin, M. E. (USSR). Tr. Perm. S.-kh. In-t (118), 57-9 From: Ref. Zh., Khim. 1976, Abstr. No. 23Zh223 (Russian) 1976.

AB Title only translated.

REFERENCE 2: 85:33073 Azaisatoic anhydrides. Beckwith, Athelstan L. J. (Sherwin-Williams Co., USA). U.S. US 3947416 19760330, 6 pp. Division of U.S. 3,887,550. (English). CODEN: USXXAM. APPLICATION: US 1969-878552 19691120.

Searched by: Mary Hale 308-4258 CM-1 12D16

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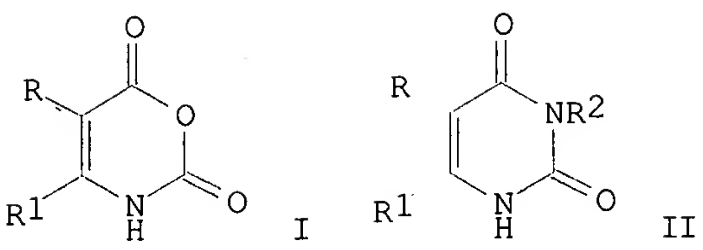


AB Isatoic anhydrides I (RR1 = CH:CHCH:CH, CH:CHCH:N, CH:CHN:CH, CH:NCH:OH) were prepd. by treating H2NCOCR1:CRCO2H with Pb(OAc)4. Pyrimidinediones II (RR1 = CH:CHCH:CH, N:CHCH:N, R2 = H, Me; RR1 = CH:CHCH:N, N:CHCH:CH, R2 = H, Bu; RR1 = CH:CHN:CH, R2 = H) were similarly obtained from R2NHCOCR1:CRCONH2 and Pb(OAc)4. I (RR1 = N:CHCH:CH, R2 = Bu) gave complete control of a variety of weeds at 16 lb./acre. II are also corrosion inhibitors.

REFERENCE 3: 85:5683 Heterocyclic acid anhydrides and pyrimidinediones. Beckwith, Athelstan L. J. (Sherwin-Williams Co., USA). U.S. US 3947442 19760330, 6 pp. Division of U.S. 3,887,550. (English). CODEN: USXXAM. APPLICATION: US 1969-878552 19691120.

AB Heterocyclic acid anhydrides e.g., 3-azaisatoic anhydride and pyrimidinediones e.g., pyrazino[2,3-d]pyrimidine-2,4(1H,3H)-dione (I), 3-butylpyrido[3,2-d]pyrimidine-2,4(1H,3H)-dione (II) were prepd. from the corresponding acids, dicarboxamides, 2,3- and 3,4-pyridinedicarboxamides by treating with Pb(OAc)4. Thus, cyclization of 2,3-pyrazinedicarboxamide with Pb(OAc)4 in DMF at 40.degree. gave 71% I. II at 16 lbs./acre gave 100% control of alfalfa, corn, wild oats etc., 70% control of lambsquarter and 90% control of crabgrass.

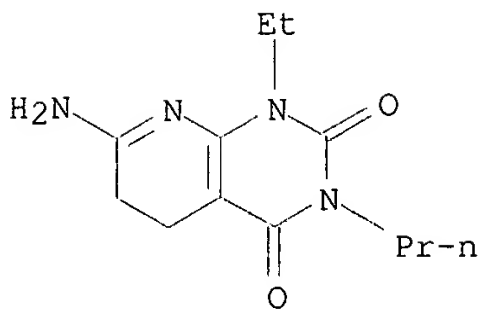
REFERENCE 4: 83:147504 Heterocyclic acid anhydrides. Beckwith, Athelstan L. J. (Sherwin-Williams Co., USA). U.S. US 3887550 19750603, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 1969-878552 19691120.

GI For diagram(s), see printed CA Issue.

AB Four acid anhydrides I (one of X, X1, or X2 is N and the rest CH) and 8 pyrimidinediones II (two of X, X1, X2, or X3 are N and the rest CH; R = H, Me, Bu), useful as herbicides, uv absorbors in suntan lotions, and corrosion inhibitors (no data), were prepd. by reaction of III (each of R1 and R2 is OH or NHR, not more than one of R1 and R2 is OH, and when either of R1 or R2 is OH, R is H, X3 is CH, and not more than one of X, X1, and X2 is N) with Pb(OAc)4. Thus, 2,3-pyridinedicarboxylic acid was dehydrated with Ac2O in AcNH2 to give 2,3-pyridinedicarboximide which reacted with BuNH2 to give N2-butyl-2,3-pyridinedicarboxamide (III, X2 = N, X, X1, X3 = CH, R1 = NH2, R2 = NHBu) (IV) and a little N3-isomer (V). A mixt. of IV and V in DMF was treated with Pb(OAc)4 to give 78:22 3-butylpyrido[3,2-d]- and 3-butylpyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione.

L3 ANSWER 22 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 13660-80-5 REGISTRY
CN Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-1-ethyl-5,6-dihydro-3-propyl- (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H18 N4 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

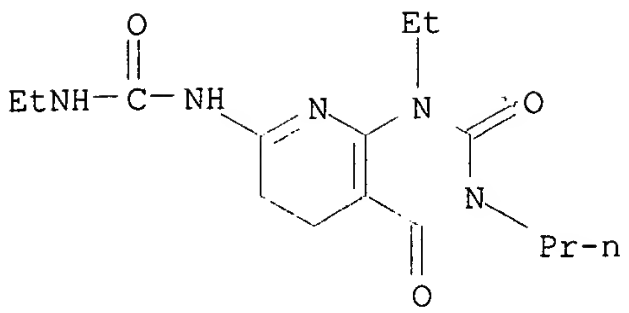
REFERENCE 1: 66:65502 7-Ureido-2,4-dioxo-1,2,3,4,5,6-hexahydropyrido[2,3-d]pyrimidines. Papesch, Viktor (Searle, G. D., and Co.). U.S. US 3296447 19670103, 3 pp. (English). CODEN: USXXAM. APPLICATION: US 19651019.

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) are prepd. by heating the corresponding 1,3-disubstituted 7-amino-2,4-dioxo-1,2,3,4,5,6-hexahydropyrido[2,3-d]pyrimidines (II) with an isocyanate in C6H6. Thus, II (R1 = R2 = Et) 5 (all quantities in parts by wt.) and EtNCO 8 in C6H6 700 parts was refluxed 20 min., the mixt. filtered, and the filtrate refluxed 1 hr. to give I (R = R1 = R2 = Et), m. 211-12.degree., resolidified 223.degree.. Other I similarly prepd. were (R, R1, R2, and m.p. given): Et, Et, Me, 202-4.degree.; Et, Et, Pr, 202-2.5.degree.; Et, Et, iso-Pr, 203-4.degree.; Et, Et, cyclohexyl, 227-8.degree.; Et, Et, allyl, 208-9.degree.; Et, Et, Ph, 224-5.degree.; Et, Et, p-tolysulfonyl, 194-5.degree.; Et, Me, Me, 295-7.degree.; Et, Me, Et, 297.degree.; Me, Et, Et, 289-92.degree.; Me, Et, iso-Pr, 297-8.degree.; Et, Pr, Et, 192-4.degree.; allyl, Et, Et, 196-7.degree.; methallyl, Me, Me, 236-8.degree.; methallyl, Me, Et, 210-12.degree.; Pr, (CH2)2CN, Et, 196-7.degree.; CH2CH2OCH2CH2CN, Et, Et, 196.degree.; EtNHCO2CH2CH2, Et, Et, 215-16.degree.. The prepn. of some II was also described. Thus, 6-amino-1-methallyl-3-methyluracil 90, 50% C5H5N-H2O (300 parts by vol.), acrylonitrile 72, and 40% aq. Me3(PhCH2)NOH (3 parts by vol.) was heated 15 min. on the steam bath, then evapd. in vacuo twice with addn. of MeOH. EtOAc was added to the residue and the mixt. filtered hot to give II (R1 = Me, R = methallyl), m. 255-7.degree.. Similarly prepd. were: II (R1 = Pr, R = Et), m. 178-9.5.degree.; II (R1 = Et, R = Me), m. 303-5.degree.; 7-amino-1,3-diethyl-4-oxo-2-thioxo-1,2,3,4,5,6-hexahydropyrido[2,3-d]pyrimidine (III), m. 228-9.degree.. III with EtNCO gave 1,3-diethyl-7-(3-ethylureido)-4-oxo-2-thioxo-1,2,3,4,5,6-hexahydro[2,3-d]pyrimidine, m. 227-8.degree.. II (R = R1 = Me) 1 was refluxed 3 hrs. with 50% Me2NCHO-C6H6 25 and EtNCO 5 parts to give I (R = R1 = Me, R2 = Et), m. >330.degree.. I are useful as hypertensive agents, esp. when R2 = Et, and are also useful as anti-ulcer agents, appetite inhibitors, antiinflammatory agents, and antibacterials effective against Bacillus subtilus and Escherichia coli.

L3 ANSWER 23 OF 23 REGISTRY COPYRIGHT 2001 ACS
RN 13660-72-5 REGISTRY
CN Urea, 1-ethyl-3-(1-ethyl-1,2,3,4,5,6-hexahydro-2,4-dioxo-3-propylpyrido[2,3-d]pyrimidin-7-yl)- (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H23 N5 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 66:65502 7-Ureido-2,4-dioxo-1,2,3,4,5,6-hexahydropyrido[2,3-d]pyrimidines. Papesch, Viktor (Searle, G. D., and Co.). U.S. US 3296447 19670103, 3 pp. (English). CODEN: USXXAM. APPLICATION: US 19651019.

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) are prepd. by heating the corresponding 1,3-disubstituted 7-amino-2,4-dioxo-1,2,3,4,5,6-hexahydropyrido[2,3-d]pyrimidines (II) with an isocyanate in C6H6. Thus, II (R1 = R2 = Et) 5 (all quantities in parts by wt.) and EtNCO 8 in C6H6 700 parts was refluxed 20 min., the mixt. filtered, and the filtrate refluxed 1 hr. to give I (R = R1 = R2 = Et), m. 211-12.degree., resolidified 223.degree.. Other I similarly prepd. were (R, R1, R2, and m.p. given): Et, Et, Me, 202-4.degree.; Et, Et, Pr, 202-2.5.degree.; Et, Et, iso-Pr, 203-4.degree.; Et, Et, cyclohexyl, 227-8.degree.; Et, Et, allyl, 208-9.degree.; Et, Et, Ph, 224-5.degree.; Et, Et, p-tolysulfonyl, 194-5.degree.; Et, Me, Me, 295-7.degree.; Et, Me, Et, 297.degree.; Me, Et, Et, 289-92.degree.; Me, Et, iso-Pr, 297-8.degree.; Et, Pr, Et, 192-4.degree.; allyl, Et, Et, 196-7.degree.; methallyl, Me, Me, 236-8.degree.; methallyl, Me, Et, 210-12.degree.; Pr, (CH2)2CN, Et, 196-7.degree.; CH2CH2OCH2CH2CN, Et, Et, 196.degree.; EtNHCO2CH2CH2, Et, Et, 215-16.degree.. The prepn. of some II was also described. Thus, 6-amino-1-methallyl-3-methyluracil 90, 50% C5H5N-H2O (300 parts by vol.), acrylonitrile 72, and 40% aq. Me3(PhCH2)NOH (3 parts by vol.) was heated 15 min. on the steam bath, then evapd. in vacuo twice with addn. of MeOH. EtOAc was added to the residue and the mixt. filtered hot to give II (R1 = Me, R = methallyl), m. 255-7.degree.. Similarly prepd. were: II (R1 = Pr, R = Et), m. 178-9.5.degree.; II (R1 = Et, R = Me), m. 303-5.degree.; 7-amino-1,3-diethyl-4-oxo-2-thioxo-1,2,3,4,5,6-hexahydropyrido[2,3-d]pyrimidine (III), m. 228-9.degree.. III with EtNCO gave 1,3-diethyl-7-(3-ethylureido)-4-oxo-2-thioxo-1,2,3,4,5,6-hexahydro[2,3-d]pyrimidine, m. 227-8.degree.. II (R = R1 = Me) 1 was refluxed 3 hrs. with 50% Me2NCHO-C6H6 25 and EtNCO 5 parts to give I (R = R1 = Me, R2 = Et), m. >330.degree.. I are useful as hypertensive agents, esp. when R2 = Et, and are also useful as anti-ulcer agents, appetite inhibitors, antiinflammatory agents, and antibacterials effective against Bacillus subtilus and Escherichia coli.

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	216.08	216.23
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-12.32	-12.32

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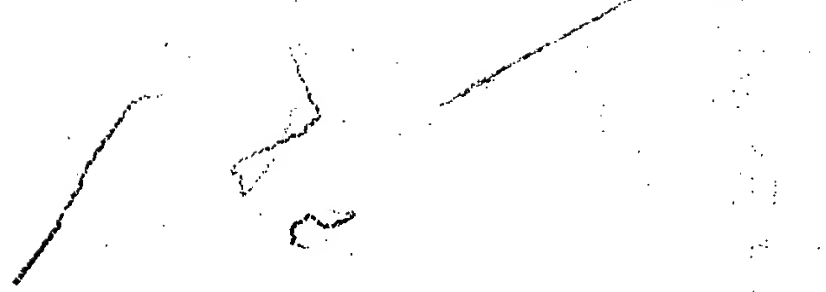

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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